Building a simple ISM model
(Glover & Mac Low 2007)

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Some basic chemistry concepts

- Chemical rate equations work in number densities. Often convenient to define n as the number density of H nuclei.

- The number density of species A is then related to the number density of H nuclei via its **abundance**, x:

$$n_A = x_A n$$

- So a gas that is full molecular (in hydrogen terms), has:

$$x_{H2} = 0.5$$

Some basic chemistry concepts

- $A^+ + BC \rightarrow AB^+ + C$ (ion-neutral)

- $A + BC \rightarrow AB + C$ (neutral-neutral)

- $A^+ + e^- \rightarrow A + \gamma$ (radiative recombination)

- $AB^+ + e^- \rightarrow A + B$ (dissociative recombination)

- $A^+ + B \rightarrow A + B^+$ (charge transfer)

- $A + B \rightarrow AB + \gamma$ (radiative association)

- $AB + \gamma \rightarrow A + B$ (photodissociation)

- $AB + \gamma \rightarrow AB^+ + e^-$ (photoionization)

WNM elemental abundances
(solar)

Abundances by number, relative to hydrogen:

Helium - 0.1

Oxygen - 3.2×10^{-4}

Carbon - 1.4×10^{-4}

Nitrogen - 7.6×10^{-4}

Sulphur - 1.2×10^{-5}

Silicon   - 1.5×10^{-5}

Reaction rates

- In a two-body reaction, we can write the reaction rate per unit volume as:

$$R_{AB} = k_{rec}\, n_A\, n_B$$

- k_{rec} is the reaction rate coefficient; n_A and n_B are the number densities of A and B

- The rate coefficient itself can be written as:

$$k_{rec} = \langle \sigma\, v \rangle$$

- σ is the reaction cross-section, v is the relative velocity of A and B, and we average over the velocity distribution

Reaction rates

- A convenient way to think of the reaction cross-section is as a product of the collision cross-section and a **reaction probability**

- Size of the collision cross-section depends on the form of the long-range inter-particle potential

- If there is no long-range force between the particles - the **hard-sphere approximation** - then σ roughly corresponds to the physical size of the target

Reaction rates

- In this case, σ is independent of velocity, which means that:

$$k_{rec} \propto v_{therm} \propto T^{1/2} \, \mu^{-1/2}$$

- If there is a long-range force between the particles, then σ can be much larger than the actual physical size of the system.

- In this case, σ typically depends on the KE of the particles, growing smaller as this increases

- In the extreme case of a Coulomb potential, we have:

$$k_{rec} \propto T^{-1/2} \, \mu^{-1/2}$$

Photodissociation

(AB + photon → A + B)

- Different chemical species photodissociate in different ways

- Why is this important? If dissociation through continuum, only effective shielding comes from dust. If dissociation through discrete lines, **self-shielding** may be important

- Self-shielding particularly effective in case of H_2: photodissociation occurs through narrow lines, and we (potentially) have lots of H_2

- In contrast, CO dissociation occurs via a wide range of fairly broad lines **and** C and O are much less abundant -- dust shielding is more effective.
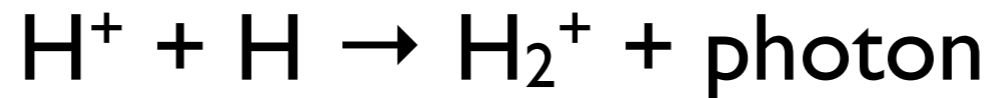
How does H$_2$ form?

- Most obvious route is via simple **radiative association**:

$$H + H \rightarrow H_2 + \text{photon}$$
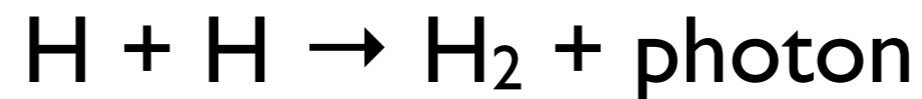
- H$_2$ has no dipole moment, and so this route is incredibly slow

- At typical ISM densities it would take longer than the age of the Universe to turn even 50% of H into H$_2$.
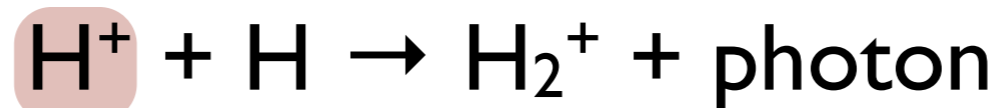
How does H$_2$ form?

- Ion-neutral reactions are more promising:

$$H + e^- \rightarrow H^- + photon$$

$$H^- + H \rightarrow H_2 + e^-$$

$$H^+ + H \rightarrow H_2^+ + photon$$

$$H_2^+ + H \rightarrow H_2 + H^+$$

- Two main problems:

  - Both chains are initiated by radiative association reactions. These are typically slow.

 - H$^-$ & H$_2^+$ are fragile -- easily destroyed by the ISRF.

How does H₂ form?

- Ion-neutral reactions are more promising:

$$H + e^- \rightarrow H^- + photon$$

$$H^- + H \rightarrow H_2 + e^-$$

$$H^+ + H \rightarrow H_2^+ + photon$$

$$H_2^+ + H \rightarrow H_2 + H^+$$

- Two main problems:

  - Both chains are initiated by radiative association reactions. These are typically slow.

  - H^- & H_2^+ are fragile -- easily destroyed by the ISRF.

How does H₂ form?

- Three body reactions (with other species) provide a means by which to remove the excess energy:

$$H + H + H \rightarrow H_2 + H$$

$$H_2 + H + H \rightarrow H_2 + H_2$$
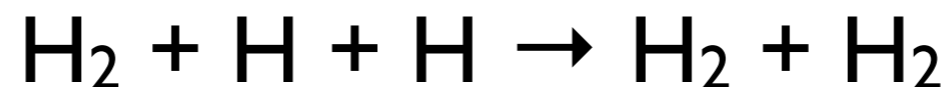
- At typical GMC/ISM densities, these reactions are slower than the ion-neutral routes.

- Become important only at high T (> 500K) and high densities (> 10^8 cm^{-3}).

- Plays an important role in primordial chemistry.

How does H_2 form?

- Formation on dust grains is actually the most effective route for forming H_2 in the ISM:

$$H + H_S \rightarrow H_2$$

- For standard MW dust properties, this process yields an H_2 formation rate of around

$$R_{H2} = 3 \times 10^{-18} \ T^{-\frac{1}{2}} \ f(T, T_{dust}) \ n \ n_H$$

- When T, and T_{dust} are small, $f(T, T_{dust}) \sim 1$

- H_2 formation timescale in the CNM (T $\sim$100K) is therefore around $\sim 10^9$ / n years.

A simple ISM model

- I have put together a simple model of the ISM, based on that found in Glover & Mac Low 2007(a).

- Follows the formation of H_2 & H^+, and main heating/cooling processes.

- The code is a subroutine that can be called for each SPH particle.

- Given the input conditions (rho, u, abundances, etc), the code will advance the particle's properties over the required timestep Δt.

- Essentially, this is a **one-zone** algorithm: for a given rho, T, etc it gives you the solution over the required Δt).

Which reactions are included?

Reaction   **References**

1. $H + H + grains \rightarrow H_2 + grains$ Hollenback & McKee (1979)
2. $H_2 + H \rightarrow 3H$ Mac Low & Shull (1986) (low density)
3. $H_2 + H_2 \rightarrow 2H + H_2$ Martin et al. (1998) (low density)
4. $H_2 + photon \rightarrow 2H$ Drain & Bertoldi (1996)
5. $H + c.r. \rightarrow H^+ + e^-$
6. $H + e^- \rightarrow H^+ + 2e^-$ Abel et al. (1997)
7. $H^+ + e^- \rightarrow H + photon$ Ferland et al. (1992)
8. $H^+ + e^- + grain \rightarrow H + grain$ Weingartner & Draine (2001)

Glover & Mac Low 2007a

What about H and e?

- The chemical rate equations also require the abundances of neutral hydrogen (H) and the electron fraction... How do we get them?

- From conservation laws:
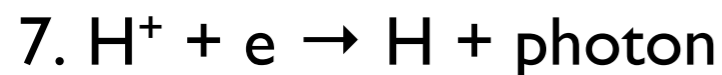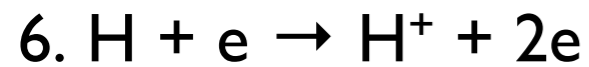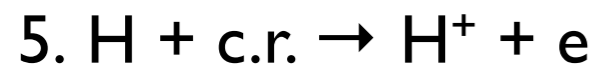
$$x_{\mathrm{H}} = 1 - 2x_{\mathrm{H_2}} - x_{\mathrm{H+}}$$
$$x_{\mathrm{e}} = x_{\mathrm{H+}} + x_{\mathrm{C}} + x_{\mathrm{Si}}$$

- Here x_{C} and x_{Si} are the relative abundances of carbon and silicon in the ISM, and we are assuming that they are both singly ionised.

- Remember that in our definition above, a gas that is fully H_2 has,

$$x_{\mathrm{H_2}} = 0.5$$

Chemical heating/cooling

Reaction	References
1. $H + H + grains \rightarrow H_2 + grains$	Hollenback & McKee (1979)
2. $H_2 + H \rightarrow 3H$	Mac Low & Shull (1986) (low density)
3. $H_2 + H_2 \rightarrow 2H + H_2$	Martin et al. (1998) (low density)
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5. $H + c.r. \rightarrow H^+ + e$	Goldsmith & Langer (1978)
6. $H + e \rightarrow H^+ + 2e$	Abel et al. (1997)
7. $H^+ + e \rightarrow H + photon$	Wolfire et al. (2003)
8. $H^+ + e + grain \rightarrow H + grain$	Wolfire et al. (2003)

Glover & Mac Low 2007a

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Glover & Mac Low 2007a

Heating and cooling in the ISM

Photoelectric emission from dust grains
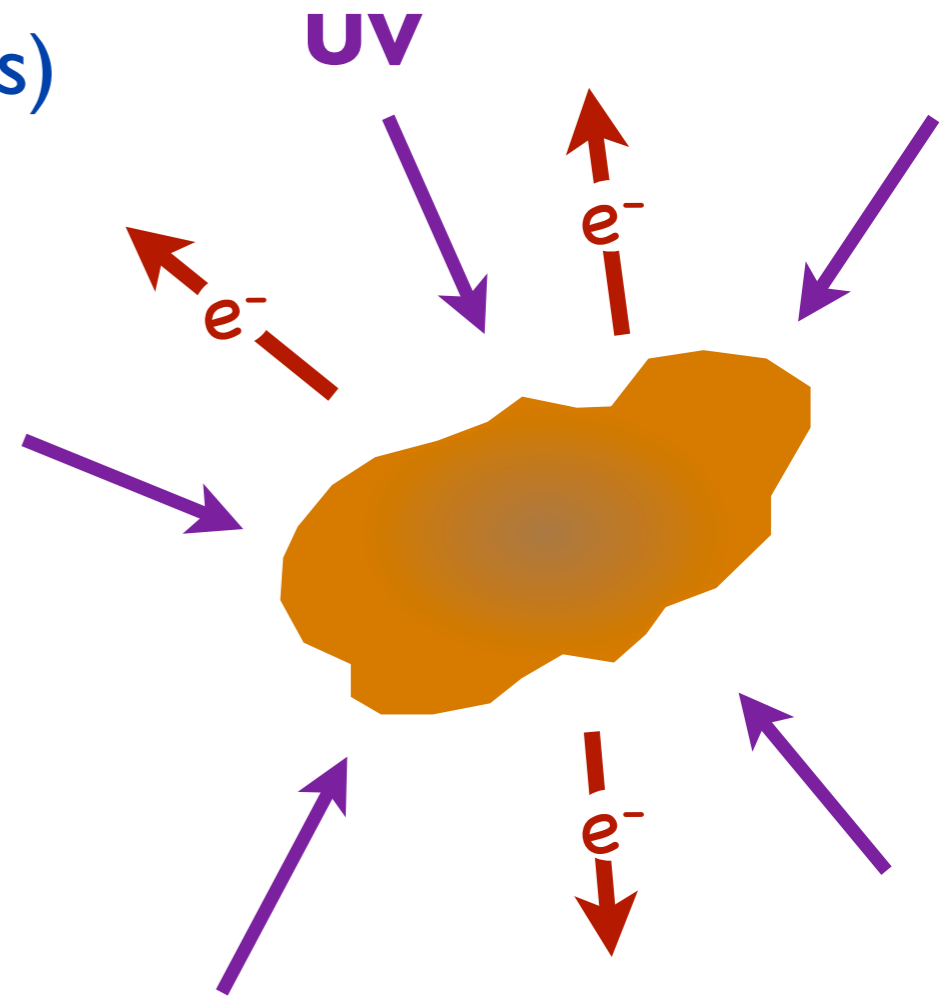
- UV radiation from the ISRF (or nearby stars) results in photoelectric emission from dust grains.

$$\Gamma_{\rm pe} = 1.3 \times 10^{-24} n\epsilon\chi_{\rm eff} \ {\rm ergs \ s}^{-1}$$

$$\chi_{\rm eff} = e^{-2.5A_{\rm V}}\chi$$

Bakes & Tielens (1994)
Wolfire et al. (2003)

- Depends on the extinction ($A_{\rm V}$) to the radiation source (position in cloud)

- There is also an efficiency factor ε, that depends on the electron fraction in the gas.

UV

e^-

e^-

e^-

How to treat the shielding?

- Reaction 4 in our network follows the destruction of H_2 by Lyman-Werner photons (11.5 to 13.6 eV).

- Also important for the photoelectric emission heating.

- Need to know the flux of these photons passing through our cell/particle.

- Depends on the column density of H_2 and dust between the source (the ISRF -- normally that of Draine 1978) and the cell.

- How to estimate?

- Simple prescription is currently implemented:

$$N = n \, L$$
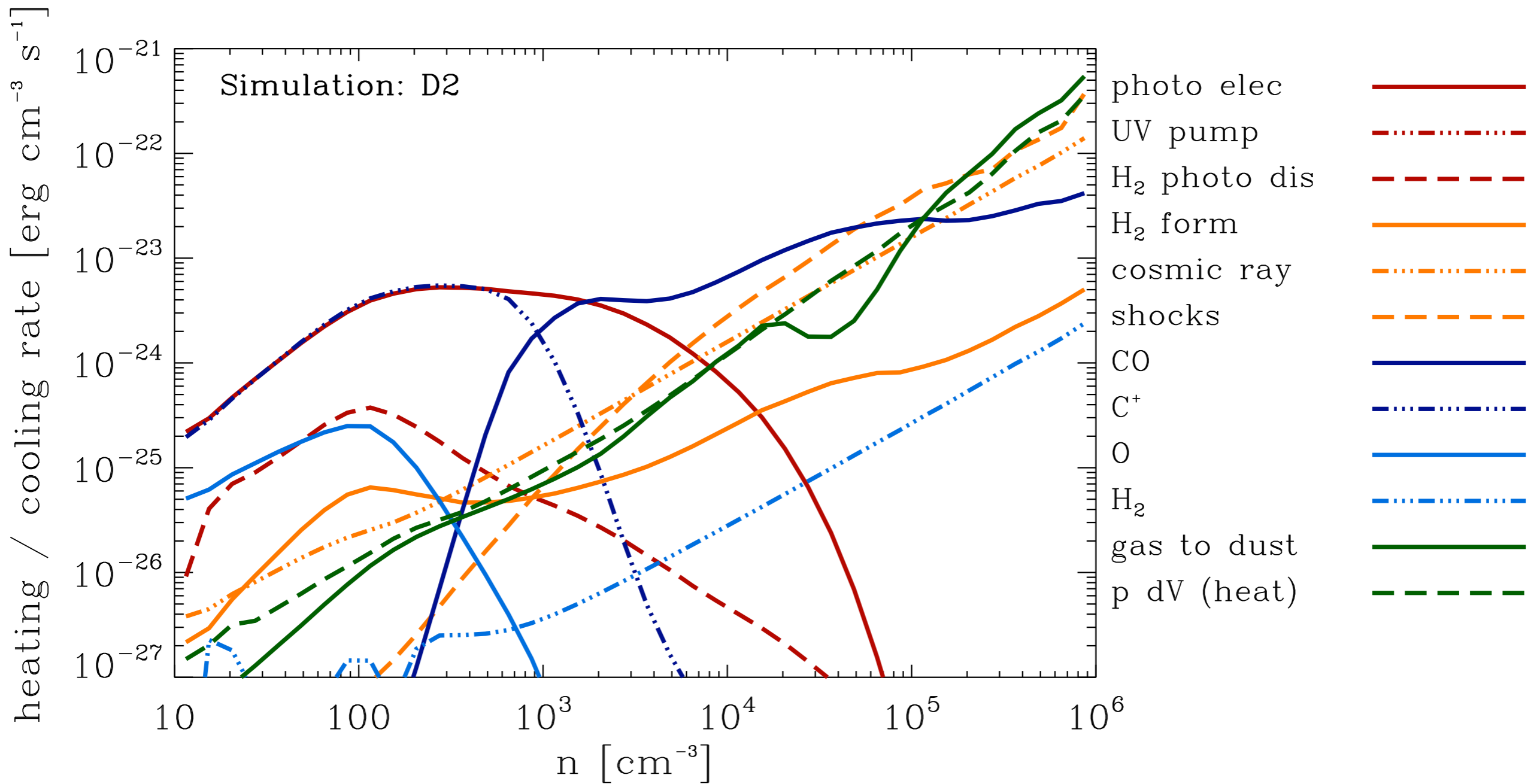
Heating and cooling in the ISM

Cooling

- Upwards of around 8000 K, the cooling is dominated by atomic resonance lines -- in this simple model, we are only considering Lyman alpha cooling (HI electronic excitation cooling). Others also contribute. A tabulated function is available from Sutherland & Dopita (1993).

- Cooling by CII and OI dominate at lower temperatures. CII tends to dominate so in our simple model, we only include it.

- In gas at high densities (n ~ 10^5 cm^{-3}), gas→grain energy transfer dominates. Use prescription from Hollenbach & McKee (1989):

$$\Lambda_{\text{gr}} = n_{\text{gr}} n \bar{\sigma}_{\text{gr}} v_{\text{p}} f (2kT - 2kT_{\text{gr}}) \ \text{erg s}^{-1} \ \text{cm}^{-3}$$

ISM heating/cooling

Simulation: D2

photo elec
UV pump
H$_2$ photo dis
H$_2$ form
cosmic ray
shocks
CO
C$^+$
O
H$_2$
gas to dust
p dV (heat)

heating / cooling rate [erg cm^{-3} s^{-1}]

n [cm^{-3}]

Glover & Clark (2012)

The equations

H$_2$ abundance:

$$n_{\mathrm{H}_2}(t_1) = \frac{n_{\mathrm{H}_2}(t_0) + C_{\mathrm{H}_2}(t_1)\Delta t}{1 + D_{\mathrm{H}_2}(t_1)\Delta t}$$

H$^+$ abundance:

$$n_{\mathrm{H}^+}(t_1) = \frac{n_{\mathrm{H}^+}(t_0) + C_{\mathrm{H}^+}(t_1)\Delta t}{1 + D_{\mathrm{H}^+}(t_1)\Delta t}$$

The energy (density):

$$e_1 = e_0 + \left[\Gamma_{\mathrm{chem}} + \Gamma_{\mathrm{ISM}} + \Lambda_{\mathrm{chem}} + \Lambda_{\mathrm{ISM}}\right]\Delta t$$

Treating the energy

Two options:

I) Operator split the energy. Evolve pdV and shocks in the code, and pass the updated e to the chemistry iterator to use as e_0 in

$$e_1 = e_0 + \left[\Gamma_{\text{chem}} + \Gamma_{\text{ISM}} + \Lambda_{\text{chem}} + \Lambda_{\text{ISM}}\right]\Delta t$$

ii) Pass the heating/cooling rates from the SPH code into the chemistry iterator and solve them with the ISM and chemistry heating/cooling rates:

$$e_1 = e_0 + \left[\Gamma_{\text{chem}} + \Gamma_{\text{ISM}} + \Lambda_{\text{chem}} + \Lambda_{\text{ISM}} + \Gamma_{\text{pdV}} + \Gamma_{\text{shock}}\right]\Delta t$$

- Pass the heating/cooling rates from the SPH code into the chemistry iterator and solve them with the ISM and chemistry heating/cooling rates:

How to solve?

(Jacobi iteration)

- Our equations have t_1 on both sides, so we need to iterate.

- Simplest way to proceed is to use the Jacobi method.

- Can be summarised as follows:

  (i) Compute the new H_2 abundance using the values at t_0

  (ii) Compute the new H^+ abundance using the values at t_0

  (iii) Compute the new energy using the values at t_0

  (iv) Update H and e^- abundances

  (v) Now go back to (i) using the new values of H_2, H^+, H and e^-, and T

How to solve?

(Gauss-Seidel iteration)

- Better, is the Gauss-Seidel method:

    (i) Compute the t_1 H_2 abundance using the values at t_0

    (ii) Update H and e^- abundances

    (iii) Compute the t_1 H^+ abundance using the new H_2, H and e^-

    (iv) Update H and e^- abundances

    (v) Compute the t_1 energy using the new values of H_2, H^+, H and e^-

    (vi) Update T

    (vii) Now go back to (i) using the new values of H_2, H^+, H and e^-

Sub-cycling

- During the timestep (Δt), the iteration may fail in a number of ways:
  - The chemical abundances fail to converge!
  - The chemical abundances want to change too rapidly over timestep Δt (i.e. greater than some pre-allowed tolerance).
  - The energy may want to change too much over Δt
  - The energy may go negative
- Simplest option is to reduce the timestep for the iteration, and try again.
- But main the SPH code wants the chemistry/thermodynamics updated over Δt for this particle.
- This is where sub-cycling comes in: keep calling the BD solver until the step Δt is complete.

Controlling the stepsize

- Particles are on different timesteps, which depend on what's happening to it.

- Ideally, we'd like to take the cooling time into consideration, to stop the code creating cold spots.

- Constrain particle's timestep to be some fraction of the "cooling time":

$$\Delta t = C_e \frac{e}{\mathrm{d}e/\mathrm{d}t}$$

- But what happens first time step? Does the code just cool/heat as much as it wants?

- Probably this is OK (equivalent to starting with a new equilibrium), but might not be good when stopping and starting the code.

- Safer is to call the chemistry for every particle at the beginning of the simulation to find the $\mathrm{d}e/\mathrm{d}t$, to get the cooling time (not implemented!).

Introduce the subroutines!

- do_chemcool_step.F90 :

  - Evolves the chemical abundances and energy for SPH particle over timestep Δt. Controls the sub-cycling of the iteration.

- solve_chem_timestep.F90 :

  - The iterative solver for the chemistry and the ISM heating/cooling.

- chemical_rate_coeff.F90:

  - Stores the reaction rate coefficients (with the exception of the cosmic-ray ionisation rate, since it requires no functional form).

# Introduce the subroutines!

In src/chemcool/

- ism_heat_cool_rate.F90 :

  - The heating and cooling from non-chemical sources (line cooling, PE heating, gas-dust cooling).

- compute_stim.F90 :

  - Computes the simulated emission for a level, given a background radiation temperature.

- chemistry_constants.F90:

  - Holds the various constants needed by the chemical model, such as metallicity, gas-to-dust ratio, as well as tolerances for the iteration scheme.

Where the chemistry appears...

- Integration scheme (currently on the KDK leapfrog):

    - File: src/advance/advance_leapfrog_kdk.F90

- Also need to modify the timestep control:

    - File: src/timestep/timestep_size.F90

- EOS and pressure calculations, etc:

    - Files: i) src/sph/thermal.F90

        ii) src/sph/thermal_properties.F90

- And also in the header file (need to add the abundances to the SPH particle structure).

Science with this setup?

- Similar in terms of included physics to the model by Dobbs et al. (2008):
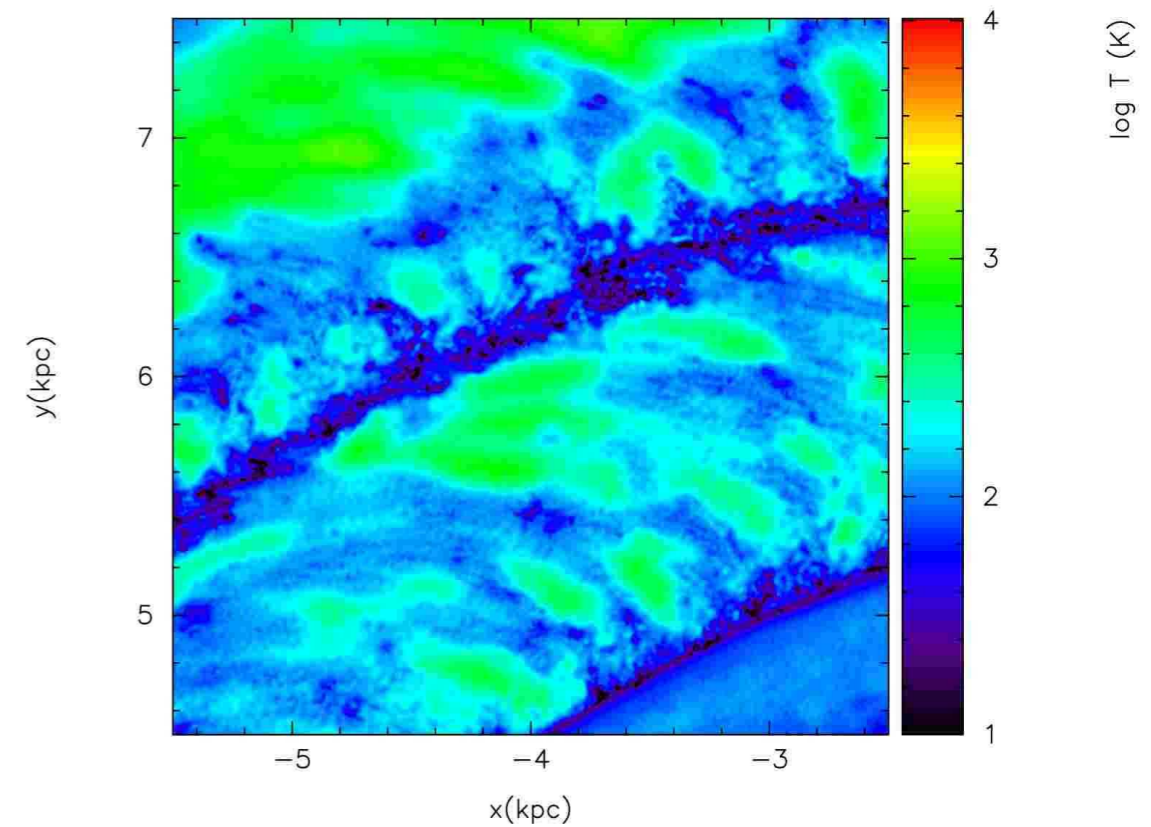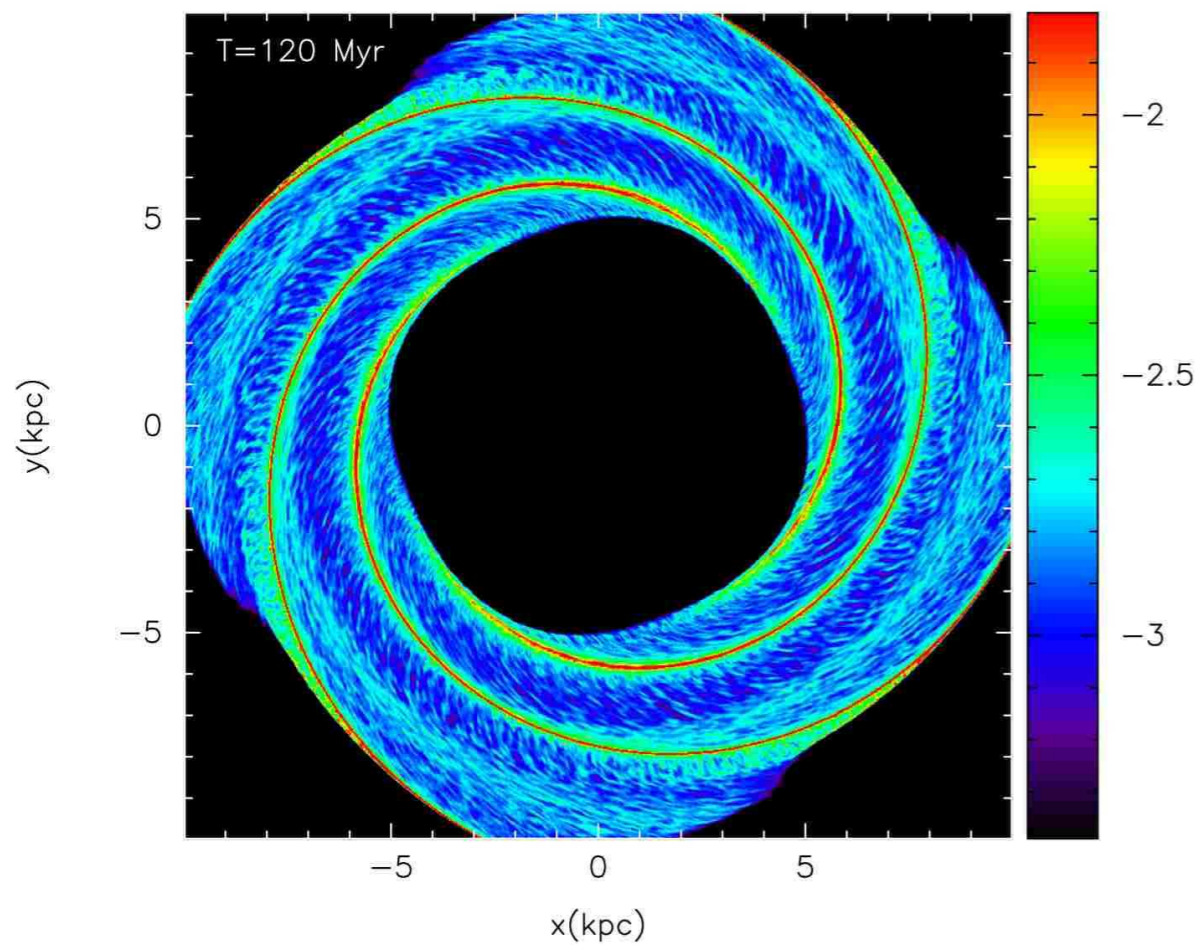
Good test case?

Test problem 1

- Possible test setup is a low-density turbulent box

- Try setting T_0 = 7000 K; n = 1 cm^{-3}; mass = 1×10^5 M$_\odot$

- Start with H$_2$ and H$^+$ abundances of 0 and ~ 0.001 respectively.

- Maybe use 1,000,000 SPH particles to start with.

- Best to use all 16 cores in the node ;-)

Good test case?

Test problem 2

- Could also try to set up 2 colliding clouds.

- Create two turbulent spheres (with $E_K \sim 0.5E_G$)

- Masses of around 1×10^5 $M_\odot$

- You will need the external pressure term.

- Collide with 10-20 km/s.